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LEAST SQUARES OVER THE COMPLEX FIELD

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LEAST SQUARES OVER THE COMPLEX FIELD

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ABSTRACT: The least square solution of a set of linear equations with complex coefficients and its relation to the equivalent real equations is discussed. In particular it is shown that the square root method of solving the normal equations is extendible to the complex field and that fewer operations are required to effect this solution by computing with complex numbers rather than with real numbers.

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This report discusses the least square solution of a set of complex linear equations. The study has been carried out as a part of Project NOL-B3d-452-1-55, entitled "Free Flight Aeroballistics," and Project FR-30-55, entitled "Numerical Analysis."

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LEAST SQUARES OVER THE COMPLEX FIELD

1. Introduction

Sets of complex linear (observational) equations in $s \leq r$ unknowns arise in ballistics. For the equivalent real equations the least square solution is frequently accomplished by the square root method. This method has several characteristics which recommend it for use with high speed computing machinery:

(1) In fixed decimal machines the scaling problem tends to be minimized because the square root operation reduces the spread of data.

(2) The algorithms involved are particularly simple and independent of the number of unknowns. (This implies that to extend a set of instructions for solving an nth order system to a larger system requires only adding instructions.)

(3) Storage allotment is systematic and simple.

(4) The amount of storage required (at least with certain machines)[1] appears to be minimal.

(5) A simple simultaneous check of the formation and solution of the normal equations and calculation of residuals is possible (cf. theorem 5).

(6) Weights[2] of the unknowns are readily calculated from intermediate results.

It is not appreciated in all computing circles that the square root technique admits of a trivial extension to the complex domain maintaining the characteristics mentioned above. Once this is appreciated it is natural to ask whether there is "any difference" in solving the complex normal equations by computing with complex numbers or by computing with

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[1] The program constructed at NOL for use on a Card Programmed Calculator using a double operation general purpose board requires no temporary storage. The storage requirement for solving a system of n equations with n unknowns is one more than the number of (in general distinct) elements in the (augmented) matrix, i.e., the storage requirement is $\frac{1}{2}(n+1)(n+2)$.

[2] See Whittaker and Robinson, Calculus of Observations, Third Edition, p. 239.

real numbers. It turns out that the number of real operations (of each type) required to solve the normal equations by computing within the complex domain is less than or equal to half the number of real operations required to solve the equations by computing within the real domain.

2. The problem

Let $M = N + iP$ be a complex $r \times s$ matrix, $s \leq r$. Let $w = u + iv$ be a complex $r \times 1$ matrix (or column vector). The problem, then, is to find a complex $s \times 1$ matrix, $z = x + iy$, which, in the least square sense, is the best possible solution to the set of equations

$$Mz \doteq w. \tag{1}$$

("$\doteq$" denotes "equals approximately" and is used to emphasize that there exists, in general, no z such that $Mz = w$ precisely.)

From (1) we obtain

$$(N + iP)(x + iy) \doteq u + iv$$

$$(Nx - Py) + i(Px + Ny) \doteq u + iv$$

so that

$$Nx - Py \doteq u \quad \text{or} \quad (N \quad -P)\begin{pmatrix} x \\ y \end{pmatrix} \doteq u \tag{2}$$

and

$$Px + Ny \doteq v \quad \text{or} \quad (P \quad N)\begin{pmatrix} x \\ y \end{pmatrix} \doteq v. \tag{3}$$

Equations (2) and (3) taken together yield

$$\begin{pmatrix} N & -P \\ P & N \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \doteq \begin{pmatrix} u \\ v \end{pmatrix}. \tag{4}$$

The two methods[3] of solving (1) with which we are familiar both seek

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[3] Cf. references 4 and 6.

the solution of (4).

3. The mapping

We note that (2) and (3) are respectively equivalent to

$$(P \quad N)\begin{pmatrix} -y \\ x \end{pmatrix} \doteq u$$

$$(N \quad -P)\begin{pmatrix} -y \\ x \end{pmatrix} \doteq -v$$

and these latter taken together are equivalent to

$$(5) \qquad \begin{pmatrix} N & -P \\ P & N \end{pmatrix}\begin{pmatrix} -y \\ x \end{pmatrix} \doteq \begin{pmatrix} -v \\ u \end{pmatrix}.$$

(4) and (5) are equivalent and each is equivalent to

$$(6) \qquad \begin{pmatrix} N & -P \\ P & N \end{pmatrix}\begin{pmatrix} x & -y \\ y & x \end{pmatrix} \doteq \begin{pmatrix} u & -v \\ v & u \end{pmatrix}.$$

Let f denote the mapping

$$f(M) = \begin{pmatrix} N & -P \\ P & N \end{pmatrix} \qquad \text{for any complex matrix } M.$$

Then (6) may be written

$$f(M)\cdot f(z) \doteq f(w).$$

4. Some theorems

Theorem 1. For any $z = x + iy$ the sum of the squares of the moduli of the residuals of (1) equals the sum of the squares of the residuals of (4).

Proof. The sum of the squares of the residuals of (1) may be written

in matrix terminology as

$$(7) \qquad {}^t(\overline{Mz - w})(Mz - w)$$

where "${}^tA$" denotes the transpose of the matrix A and $\bar{A}$ denotes the matrix obtained from A by replacing each element by its conjugate. [For ${}^t\bar{A}$ we shall often write $*A$.] Replacing M by N + iP, z by x + iy and w by u + iv we obtain

$$Mz - w = (Nx - Py - u) + i(Px + Ny - v)$$

so that (7) becomes

$$(8) \qquad {}^t(Nx - Py - u)(Nx - Py - u) + {}^t(Px + Ny - v)(Px + Ny - v).$$

The sum of the squares of the residuals of (4) is

$$^t\left|\begin{pmatrix} N & -P \\ P & N \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} u \\ v \end{pmatrix}\right|\left|\begin{pmatrix} N & -P \\ P & N \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} u \\ v \end{pmatrix}\right|$$

$$= {}^t\begin{pmatrix} Nx - Py - u \\ Px + Ny - v \end{pmatrix}\begin{pmatrix} Nx - Py - u \\ Px + Ny - v \end{pmatrix}$$

which equals (8) and hence (7).

<u>Lemma 1.</u> If A is a hermitian positive definite matrix, then there exists at most one triangular matrix S with real positive diagonal elements such that ${}^t\bar{S}\cdot S = A$. ($S = (s_{ij})$ is triangular shall mean that S is a square matrix with the property that $i > j$ implies $s_{ij} = 0$.)

<u>Proof.</u> Assuming S exists we have $\sum_{k=1}^{n} \bar{s}_{ki}s_{kj} = a_{ij}$, $1 \leq i,j \leq n$, where n is the order of A. Since $i > j$ implies $s_{ij} = 0$, for $i \leq j$ we have $a_{ij} = \sum_{k=1}^{i} \bar{s}_{ki}s_{kj}$, which yields the formulas:

$$s_{11} = \sqrt{a_{11}}, \qquad s_{1j} = \frac{a_{1j}}{s_{11}}, \quad 1 < j \leq n,$$

(9) $$s_{ij} = (a_{ij} - \sum_{k=1}^{i-1} \bar{s}_{ki}s_{kj})/s_{ii}, \quad 1 < i < j \leq n,$$

$$s_{jj} = \sqrt{a_{jj} - \sum_{k=1}^{j-1} \bar{s}_{kj}s_{kj}}, \quad 1 < i = j \leq n.$$

Theorem 2. The following five conditions on a hermitian $n \times n$ matrix A are equivalent. [(a) is taken as the definition of a matrix being positive definite.]

(a) ${}^t\bar{x}Ax > 0$ for all non-zero complex $n \times 1$ matrices x.[4]

(b) $A = {}^t\bar{B}\cdot B$ for some complex $r \times s$ matrix B and $|A| \neq 0$.

(c) The principal minors of A are all positive, i.e., the determinants of all matrices obtained from A by deleting the same rows and columns are all positive. ($|A|$ is a principal minor.)

(d) $A = {}^t\bar{S}\cdot S$ for a complex triangular matrix $S = (s_{ij})$ with positive diagonal elements.

(e) Let A_i, $1 \leq i < n$, denote the matrix obtained from A by deleting rows and columns $i + 1, i + 2, \cdots, n$. $|A_i| > 0$ for $1 \leq i < n$ and $|A| > 0$.

Proof. (a) implies (e). Let $\lambda_1, \lambda_2, \cdots, \lambda_n$ be the not necessarily distinct roots (eigenvalues) of $g(\lambda) = |A - \lambda I|$, so that $g(\lambda) = \prod_{i=1}^n (\lambda_i - \lambda)$. Then $g(0) = |A| = \prod_{i=1}^n \lambda_i$. For each λ_i there exists a non-zero n-tuple (column vector, eigenvector) x_i such that $Ax_i = \lambda_i x_i$, since there exists a non-trivial (non-zero) solution to the equations

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(4) For any hermitian A, $\overline{{}^t\bar{x}Ax} = {}^tx\bar{A}\bar{x} = {}^t({}^t\bar{x}\bar{A}\bar{x})$ … $= {}^t\bar{x}\,{}^t\bar{A}x = {}^t\bar{x}Ax$ so that ${}^t\bar{x}Ax$ is real.

$(A - \lambda_i I)x = 0$. Using the hypothesis: ${}^t\bar{x}_i \cdot Ax_i = {}^t\bar{x}_i \cdot \lambda_i x_i = \lambda_i \cdot {}^t\bar{x}_i x_i > 0$, so that $\lambda_i > 0$. Hence $|A| = \prod_{i=1}^{n} \lambda_i > 0$.

Let $A(i)$ denote the matrix obtained from A by deleting the ith row and column and $x(i)$ the column matrix obtained from the n x 1 matrix x by deleting the ith element (row). If the ith row of x is zero, then

$$ {}^t\bar{x}Ax = {}^t\overline{x(i)}\, A(i)\, x(i), $$

so that $A(i)$ is positive definite. From the preceding paragraph, $|A(i)| > 0$. It follows that all principal minors are positive.

(c) implies (e). Obvious.

(e) implies (d). $|A_1| = a_{11} > 0$, so that there exists $s_{11} = \sqrt{a_{11}}$ and $s_{12} = a_{12}/s_{11}$. If $a_{22} - \bar{s}_{12}s_{12} > 0$, then we can find $s_{22} > 0$ and s_{13}, s_{23} satisfying (9) above. If, further, $a_{33} - \bar{s}_{13}s_{13} - \bar{s}_{23}s_{23} > 0$, then we can find $s_{33} > 0$, s_{14}, s_{24}, s_{34} satisfying (9) above. Let r denote the least j such that

$$ a_{jj} - \sum_{k=1}^{j-1} \bar{s}_{kj}s_{kj} \leq 0 \tag{10} $$

(assuming there exists such a j, $1 < j \leq n$). Let $s_{rr} \geq 0$ be such that

$$ -s_{rr}^2 = a_{rr} - \sum_{k=1}^{r-1} \bar{s}_{kr}s_{kr}. $$

Denoting the triangular matrix $(s_{ij})_{1 \leq i,j \leq r}$ by S_r we have

$$ \tilde{S}_r \cdot S_r = A_r $$

where $\tilde{S}_r$ is ${}^t\bar{S}$ except in the rth row and column stands $-s_{rr}$ instead of s_{rr},

$$ |S_r| = \prod_{i=1}^{r} s_{ii}, $$

$$ |\tilde{S}_r| = -\prod_{i=1}^{r} s_{ii}, $$

so that

$$|A_r| = -\prod_{i=1}^{r} s_{ii}^2.$$

The left-hand member is positive by hypothesis, while the right-hand member is negative or zero. Thus the assumption of the existence of j, $1 < j \leq n$, such that (10) holds is false, and the existence of S is established.

(d) implies (b). Take $B = S$. $|A| > 0$ since $|A| = \prod_{i=1}^{n} s_{ii}^2$ and $s_{ii} > 0$.

(b) implies (a). ${}^t\bar{x}Ax = {}^t\bar{x}\cdot{}^t\bar{B}B\cdot x = {}^t\bar{x}\,{}^t\bar{B}\cdot Bx = {}^t(\overline{Bx})Bx \geq 0$ since ${}^t(\overline{Bx})Bx$ is a sum of squares. If, for some x, ${}^t(\overline{Bx})Bx = 0$, then $Bx = 0$. Hence ${}^t\bar{B}\cdot Bx = Ax = 0$. $|A| \neq 0$ and $Ax = 0$ imply $x = 0$ (this follows from Cramer's rule).

<u>Corollary</u>. If A is hermitian positive definite, then there exists a unique triangular matrix with positive diagonal elements such that

$$A = {}^t\bar{S}\cdot S.$$

<u>Proof</u>. Immediate from lemma 1 and theorem 2.

<u>Lemma 2</u>. If the sum (product) of two complex matrices M_1, M_2 is defined, then the sum (product) of the two real matrices $f(M_1)$, $f(M_2)$ is defined and

(a) $f(M_1 + M_2) = f(M_1) + f(M_2)$,

(b) $f(M_1 \cdot M_2) = f(M_1)\cdot f(M_2)$,

(c) $f(aM) = af(M)$ for any real number a.

<u>Proof</u>. That the sum and product of $f(M_1)$, $f(M_2)$ are defined is clear. Proofs of (a) and (c) are obvious.

(b) Let $M_1 = N_1 + iP_1$, $M_2 = N_2 + iP_2$. Then

$$f(M_1)\cdot f(M_2) = \begin{pmatrix} N_1 & -P_1 \\ P_1 & N_1 \end{pmatrix}\begin{pmatrix} N_2 & -P_2 \\ P_2 & N_2 \end{pmatrix}$$

$$= \begin{pmatrix} N_1N_2 - P_1P_2 & -(N_1P_2 + P_1N_2) \\ N_1P_2 + P_1N_2 & N_1N_2 - P_1P_2 \end{pmatrix}$$

$$= f(M_1\cdot M_2).$$

Remark. An n x n matrix A is called non-singular if A^{-1} exists. A^{-1} exists if and only if $|A| \neq 0$ since (1) if A^{-1} exists, $A\cdot A^{-1} = I$, $|A|\cdot|A^{-1}| = 1$, so that $|A| \neq 0$, and (2) if $|A| \neq 0$, then $Ab_{ij} = \delta_{ij}$, $1 \leq i \leq n$, fixed j, has a solution by Cramer's rule; let j vary between 1 and n, then if $B = (b_{ij})$, $AB = I$.

Lemma 3. (a) $f(I_n) = I_{2n}$, where I_n denotes the n x n identity matrix.

(b) If M is a square matrix and M^{-1} exists, then f(M) is square, $[f(M)]^{-1}$ exists, and $f(M^{-1}) = [f(M)]^{-1}$.

(c) $f({}^tM) = {}^tf(M)$.

(d) $H = P + iQ$ is hermitian if and only if P is symmetric and Q is skew-symmetric.

(e) If H is hermitian positive definite, then f(H) is symmetric positive definite and if $H = P + iQ$ then P is positive definite.

Proof. (a) follows from the definition of f.

(b). If $AM = I$, then $f(A)\cdot f(M) = I$ using lemma 2(b) and lemma 3(a). Thus $f(A) = (f(M))^{-1}$ if $A = M^{-1}$.

(c). If $M = N + iP$, ${}^*M = {}^tN - i{}^tP$,

$$f(M) = \begin{pmatrix} N & -P \\ P & N \end{pmatrix},$$

$$f(*M) = \begin{pmatrix} {}^tN & {}^tP \\ -{}^tP & {}^tN \end{pmatrix},$$

and the result follows.

(d). Immediate from the definition of hermitian.

(e). By the corollary to theorem 2 there exists a triangular matrix S such that $*S \cdot S = H$. Applying f to both sides of this equality yields

$$f(*S) \cdot f(S) = f(H).$$

By lemma 3(c), $f(*S) = {}^tf(S)$, so that

(A) $$^tf(S) \cdot f(S) = f(H),$$

and

(B) $$^tf(H) = {}^t[{}^tf(S) \cdot f(S)] = f(H).$$

(B) shows that f(H) is symmetric. That $|f(H)| \neq 0$[5] follows from lemma 3(b). $|f(H)| \neq 0$ and (A) prove that f(H) is positive definite (over the complex numbers) by theorem 2.

Alternatively, f(H) may be proved symmetric positive definite as follows. $f(H) = \begin{pmatrix} P & -Q \\ Q & P \end{pmatrix}$. From (d), f(H) is symmetric. Since H is positive definite,

$$^t\bar{z}Hz = a(z) > 0,$$

$$^tf(z)\ f(H)\ f(z) = \begin{pmatrix} a(z) & 0 \\ 0 & a(z) \end{pmatrix} = \begin{pmatrix} {}^tx & {}^ty \\ -{}^ty & {}^tx \end{pmatrix} f(H) \begin{pmatrix} x & -y \\ y & x \end{pmatrix}$$

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[5] Indeed, it may be shown that $|f(H)| = |H|^2$.

where $z = x + iy$. It follows that

$$({}^t x \quad {}^t y)\, f(H) \begin{pmatrix} x \\ y \end{pmatrix} = a(z) > 0.^{(6)}$$

Let $S = U + iV$. Then

$$f(H) = \begin{pmatrix} P & -Q \\ Q & P \end{pmatrix} = \begin{pmatrix} {}^tU & {}^tV \\ -{}^tV & {}^tU \end{pmatrix} \begin{pmatrix} U & -V \\ V & U \end{pmatrix}.$$

It follows that $P = {}^tU \cdot U$. U is triangular and the elements along its main diagonal are the elements along the main diagonal of S. Thus $|U| = |S| \neq 0$. Therefore, P is positive definite.

Theorem 3. Assuming $|{*M} \cdot M| \neq 0$,(7) the z which minimizes the sum of the squares of the moduli of the residuals of (1) is the solution to the equation

$$(11) \qquad {*M} \cdot M \cdot z = {*M} \cdot w.$$

Proof. Since $|{*M} \cdot M| \neq 0$, it follows that $|f({*M} \cdot M)| \neq 0$ from lemma 3(b). By theorem 1, if $\begin{pmatrix} x \\ y \end{pmatrix}$ is the least square solution to (4), then $z = x + iy$ minimizes the sum of the squares of the moduli of the residuals of (1). The least square solution to (4) is the solution to the equation

$$(12) \qquad {}^t f(M) \cdot f(M) \begin{pmatrix} x \\ y \end{pmatrix} = {}^t f(M) \begin{pmatrix} u \\ v \end{pmatrix}.$$

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(6) This latter proof shows that $f(H)$ is positive definite over the real numbers. It may readily be shown that in general if a symmetric matrix is positive definite over the real numbers, it is positive definite over the complex numbers.

(7) If M is an $r \times s$ matrix, $s \leq r$, of rank s, it may be shown that $|{*M} \cdot M| \neq 0$.

Application of f to (11) yields

$$ (13) \qquad {}^{t}f(M)\cdot f(M)\cdot f(z) \;=\; {}^{t}f(M)\cdot f(w). $$

The first column of $f(z)$ is then the solution to (12) and the theorem is proved.

<u>Theorem 4</u>. Let $Ax = g$ represent a set of n linear equations in n unknowns. Assume A is an $n \times n$ hermitian positive definite matrix and g is an $n \times 1$ complex matrix. Then

(a) there exists α such that if $B = \begin{pmatrix} A & -g \\ -{}^{t}\bar{g} & \alpha \end{pmatrix}$, then $|B| = |A|$;

(b) there exist an $n \times n$ triangular matrix S and an $n \times 1$ matrix k such that

$$ \begin{pmatrix} A & -g \\ -{}^{t}\bar{g} & \alpha \end{pmatrix} = \begin{pmatrix} {}^{t}\bar{S} & 0 \\ -{}^{t}\bar{k} & 1 \end{pmatrix} \begin{pmatrix} S & -k \\ 0 & 1 \end{pmatrix}; $$

(c) there exist an $n \times n$ triangular matrix T and an $n \times 1$ matrix y such that

$$ \begin{pmatrix} \overset{n\times n}{T} & \overset{n\times 1}{y} \\ \overset{1\times n}{0} & \overset{1\times 1}{1} \end{pmatrix} \begin{pmatrix} \overset{n\times n}{S} & \overset{n\times 1}{-k} \\ \overset{1\times n}{0} & \overset{1\times 1}{1} \end{pmatrix} = \begin{pmatrix} \overset{n\times n}{I} & \overset{n\times 1}{0} \\ \overset{1\times n}{0} & \overset{1\times 1}{1} \end{pmatrix}; $$

(d) $Ay = g$.

<u>Proof</u>. Expand $|B|$ by elements of the last column, giving $|B| = c + |A|\alpha$ where c is independent of α, i.e., $|B|$ is a linear function of α. Since $|A| \neq 0$, α can be determined so that $|B| = |A|$.

Since $|B| = |A| > 0$, and A is positive definite, it follows from theorem 2, condition (e) that B is positive definite. By the corollary to theorem 2, there exists a unique $(n+1) \times (n+1)$ triangular matrix which

decomposes B (in the sense of the corollary). Since $|B|/|A|$ equals the square of the element in the (n+1)th row and column, this element is 1. Thus B decomposes as shown in (b).

Let

$$\begin{pmatrix} \overset{n\times n}{T} & \overset{n\times 1}{y} \\ \overset{1\times n}{w} & \overset{1\times 1}{1}\end{pmatrix}\begin{pmatrix} \overset{n\times n}{S} & \overset{n\times 1}{-k} \\ \overset{1\times n}{0} & \overset{1\times 1}{1}\end{pmatrix} = \begin{pmatrix} \overset{n\times n}{I} & \overset{n\times 1}{0} \\ \overset{1\times n}{0} & \overset{1\times 1}{1}\end{pmatrix}.$$

Assume inductively that T is triangular. Then $wS + 0\cdot 1 = 0$. Since $|S| \neq 0$, $w = 0$, so that the inverse of a triangular matrix is triangular. (c) follows.

From (c), $T(-k) + y\cdot 1 = 0$ and $TS = I$, so that

$$y = Tk$$

$$Sy = STk = k$$

$${}^t\bar{S}Sy = {}^t\bar{S}k.$$

From (b), $A = {}^t\bar{S}S$ and $-g = {}^t\bar{S}(-k) + 0\cdot 1$, so that (d) follows.

<u>Theorem 5</u>. Let $e = Mz - w$ where M, w are as in (1) and z is the solution to (11). Let $A = {}^*M\cdot M$ be non-singular. Let $g = {}^*M\cdot w$. Let $A = {}^*S\cdot S$, the unique triangular decomposition given by the corollary to theorem 2. Let $k = {}^*S^{-1}\, g$. Then

(14) $$ {}^*e\cdot e = {}^*w\cdot w - {}^*k\cdot k.$$

<u>Proof</u>. ${}^*e\cdot e = {}^*z{}^*MMz - {}^*wM\cdot z - {}^*z\cdot{}^*Mw + {}^*ww = {}^*z\cdot{}^*SSz - {}^*gz - {}^*zg + {}^*ww = {}^*zg - {}^*gz - {}^*zg + {}^*ww = {}^*ww - {}^*gz$. Now $Sz = k$, so that $z = S^{-1}k$, while ${}^*Sk = g$, so that ${}^*g = {}^*kS$. (14) follows.

5. <u>Weights</u>

Let A be a non-singular s x s matrix. If (x_k), $k = 1,2,\cdots,s$, is the solution of the real matrix equation

(15) $$Ax = g,$$

then the weight[8] of the solution x_k, written $w_k(x)$ or more properly $w_k(A)$, is given by

(16) $$\frac{1}{w_k(x)} = \frac{|A_k|}{|A|} = e_{kk}$$

where $|A_k|$ is the minor of a_{kk} and where $(e_{ij}) = E = A^{-1}$.

If $(z_k) = (x_k + iy_k)$, $k = 1,2,\cdots,s$, is the solution of the complex matrix equation

(17) $$Az = g$$

and

(18) $$A = B + Ci, \qquad g = m + ni,$$

then we define

(19) $$\frac{1}{w_k(A)} = \frac{1}{w_k(z)} = \frac{|A_k|}{|A|} = e_{kk}$$

and we define $w_k(x) = w_k(f(A))$ and $w_k(y) = w_{k+s}(f(A))$.

<u>Theorem 6</u>. If A is hermitian, then $w_k(z) = w_k(x) = w_k(y)$.

<u>Proof</u>. Let $A^{-1} = M + Ni$. Since A is hermitian, A^{-1} is also hermitian[9] so that N is skew-symmetric. Thus

(20) $$\frac{1}{w_k(z)} = m_{kk} + n_{kk}i = m_{kk}.$$

It follows from lemma 3(b) that

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[8]Cf. Whittaker and Robinson, Calculus of Observations.

[9]From $AA^{-1} = I$ follows $*A^{-1} \cdot *A = *(AA^{-1}) = *I = I$. $A = *A$, so that $*A^{-1} \cdot A = I$. Hence $*A^{-1} = A^{-1}$ and A^{-1} is hermitian.

$$\begin{pmatrix} B & -C \\ C & B \end{pmatrix}^{-1} = \begin{pmatrix} M & -N \\ N & M \end{pmatrix}$$

so that

$$\frac{1}{w_k(x)} = \frac{1}{w_k(y)} = m_{kk} \geq \frac{1}{w_k(z)} .$$

6. Counting operations

__Theorem 7__. Let $a(n)$, $m(n)$, $d(n)$ represent the number of real additions (or subtractions), multiplications, and divisions, respectively, required to find S such that $*S \cdot S = A$ by means of algorithm (9) on page 5 where A is a real symmetric positive definite $n \times n$ matrix and S is a triangular matrix. Let $a^{-1}(n)$, $m^{-1}(n)$, $d^{-1}(n)$ represent the number of additions (or subtractions), multiplications, and divisions, respectively, required to find $T = S^{-1}$ by means of the formulas given below. Let $*a(n)$, $\cdots$, $*a^{-1}(n)$, $\cdots$ have corresponding meanings in the case that A is a not real hermitian positive definite matrix. Then

(A)
$$a(n) = m(n) = m^{-1}(n) = \tfrac{1}{6}\, n(n^2 - 1)$$
$$d(n) = \tfrac{1}{2}\, n(n - 1)$$
$$a^{-1}(n) = \tfrac{1}{6}\, n(n - 1)(n - 2)$$
$$d^{-1}(n) = \tfrac{1}{2}\, n(n + 1),$$

(B)
$$*a(n) = *m(n) = *m^{-1}(n) = \tfrac{1}{3}\, n(n - 1)(2n - 1)$$
$$*a^{-1}(n) = \tfrac{2}{3}\, n(n - 1)(n - 2)$$
$$*d(n) = n(n - 1)$$
$$*d^{-1}(n) = n^2.$$

Proof. We establish the formulas for $m(n)$ and $*m(n)$ only. The others may be established in a similar manner. We give first the formulas for computing $T = (t_{ij})$.

$$(21) \qquad t_{jj} = \frac{1}{s_{jj}}; \qquad t_{ij} = \frac{-\sum_{k=i}^{j-1} t_{ik} s_{kj}}{s_{jj}} \quad \text{when } i < j.$$

The formula for $m(n)$ is correct for $n = 1$. Assume it correct for n. Since the number of multiplications required to compute $s_{i,n+1}$, $0 < i \leq n+1$, is $i - 1$, $m(n+1) = \frac{1}{6}n(n^2-1) + (0 + 1 + 2 + \cdots + n) = \frac{1}{6}n(n^2-1) + \frac{1}{2}n(n+1) = \frac{1}{6}n(n+1)(n+2)$, which establishes the formula.

Multiplication of two (in general unrelated and not real) complex numbers requires four real multiplications. In case of multiplication of a complex number by its conjugate, the number of real multiplications required is two. The number of multiplications required to calculate the diagonal elements (in the real case) is $\frac{1}{2}n(n-1)$. Hence $*m(n) = 4[m(n) - \frac{1}{2}n(n-1)] + 2[\frac{1}{2}n(n-1)]$, which yields the desired result.

Corollary. If A is hermitian positive definite, then the number of operations required to compute S such that $*S \cdot S = A$ is less than half that required to compute S such that ${}^tS \cdot S = f(A)$.

Proof. Let

$$\begin{aligned}
(a) &= m(2n) + m^{-1}(2n) = \tfrac{2}{3}n(2n-1)(2n+1) \\
(a)' &= *m(n) + *m^{-1}(n) = \tfrac{2}{3}n(2n-1)(n-1) \\
(b) &= a(2n) + a^{-1}(2n) = \tfrac{1}{3}n(2n-1)(4n-1) \\
(b)' &= *a(n) + *a^{-1}(n) = \tfrac{1}{3}n(n-1)(4n-5) \\
(c) &= d(2n) + d^{-1}(2n) = 4n^2 \\
(c)' &= *d(n) + *d^{-1}(n) = n(2n-1).
\end{aligned}$$

It is readily seen that

$$(a)' < \frac{1}{2}(a)$$

$$(b)' < \frac{1}{2}(b)$$

$$(c)' < \frac{1}{2}(c).$$

It is also clear that the number of square roots to be taken is 2n in the real case and n in the complex case.

7. Miscellaneous remarks

1. If λ is a real eigenvalue of A with eigenvector $z = x + iy \neq 0$, then λ is an eigenvalue of $f(A)$ with linearly independent eigenvectors $\begin{pmatrix} x \\ y \end{pmatrix}$, $\begin{pmatrix} -y \\ x \end{pmatrix}$ since $Az = \lambda z$ implies $f(A)\cdot f(z) = \lambda f(z)$. It may be noted that $x + iy$ and $-y + ix$ are linearly dependent (over the complex numbers).

2. A computing technique to solve $Az = g$ with hermitian positive definite A may be based upon the following equations

$$*S\cdot Sz = g$$
$$Sz = k \quad \text{where } k = *S^{-1} g,$$

which yields the formulas for z_i:

$$\sum_{k=i}^{n} s_{ik} z_k = k_i.$$

Thus $s_{nn} z_n = k_n$, $s_{n-1,n-1} z_{n-1} + s_{n-1} z_n = k_{n-1}$, etc.

The formulas for computing S and k are given by (9) where the last column (from left to right) of S plays the role of k.

3. It should be noted in a computation based upon theorem 4, α need not be calculated.

A variant of theorem 4, frequently convenient, is obtained by

replacing $-g$ by g, $-{}^t\bar{g}$ by ${}^t\bar{g}$, $-k$ by k, $-{}^t\bar{k}$ by ${}^t\bar{k}$ and replacing 1 by -1. y remains unchanged and $Ay = g$.

4. A computation based upon remark 3 rather than remark 2 is more economical when the weights of the unknowns are desired since the weights are the diagonal elements of A^{-1} (excluding -1), S^{-1} is calculated, and $A^{-1} = S^{-1} \cdot {}^*S^{-1}$. If the weights are not desired, a computation based on remark 2 is more economical.

5. It is frequently desirable to "scale" the $r \times s$ matrix of observational equations

$$(A) \qquad Mz \doteq w.$$

This is accomplished by considering instead of (A)

$$(B) \qquad MD\tilde{z} \doteq c \cdot w,$$

where D is an $s \times s$ diagonal matrix and c is a real number. The normal equations corresponding to (B) are $D \cdot {}^*M \cdot M \cdot D\tilde{z} = D \cdot {}^*M \cdot cw = cD \cdot {}^*Mw$ or

$$(C) \qquad DAD\tilde{z} = cDg$$

where $A = {}^*M \cdot M$ and $g = {}^*M \cdot w$. The solution to (C) is

$$\tilde{z} = D^{-1}A^{-1}D^{-1} \cdot cDg = cD^{-1} \cdot A^{-1}g$$

so that

$$\tilde{z} = cD^{-1}z$$

or

$$z = c^{-1}D \cdot \tilde{z}.$$

6. If we define $M_1 \odot M_2 = {}^*M_1 \cdot M_2$, then $A = S \odot S$, whence the name "square root method". Cf. references 1 and 2.

7. Concerning theorem 4, a convenient order of computation is s_{11}, s_{12}, s_{22}, s_{13}, s_{23}, s_{33}, $\cdots$. After s_{ij} is computed, it displaces a_{ij} in memory (the real part of s_{ij} displacing the real part of a_{ij} and the imaginary part of s_{ij} displacing the imaginary part of a_{ij}). Comparing (9), one notes that each quantity required to compute s_{ij} is in storage at the time that s_{ij} is being computed.

Similarly, a convenient order of computation for t_{ij} is t_{11}, t_{12}, t_{22}, t_{13}, t_{23}, t_{33}, $\cdots$. After t_{ij} is computed, it displaces s_{ij} in memory. Comparing (21), one notes that each quantity required to compute t_{ij} is in storage at the time that t_{ij} is being computed.

8. If H is hermitian positive definite and $H = {}^*S \cdot S$, then $f(H) = {}^t f(S) \cdot f(S)$, but $f(S)$ is not triangular. The economy of working within the complex field can be attained working in the real field if one seeks a decomposition for $f(H)$ of the above form rather than a triangular decomposition. The triangular decomposition does not make use of the special form of $f(H)$.

9. If A is a symmetric matrix and ${}^t xAx = 0$ for all real x, then $A = 0$. For, taking x to be the column matrix with 1 in the ith position and zero elsewhere yields ${}^t xAx = a_{ii} = 0$. Taking x to be the column matrix with 1 in the ith and jth positions and zero elsewhere yields ${}^t xAx = a_{ii} + 2a_{ij} + a_{jj} = 2a_{ij} = 0$ which justifies the assertion.

If H is a hermitian matrix and ${}^* zHz = 0$ for complex n x 1 matrices z, then ${}^t x\, f(H)\, x = 0$ for real 2n x 1 matrices x. It follows that $f(H) = 0$. Hence, $H = 0$.

10. Any complex matrix A may be written as

$$H_1 + iH_2$$

where $H_1 = \frac{1}{2}(A + {}^*A)$ and $H_2 = \frac{1}{2i}(A - {}^*A)$ are hermitian. If ${}^*zAz$ is real for all z, then ${}^*zH_1z + i{}^*zH_2z$ is real. By footnote 4, ${}^*zH_1z$ and ${}^*zH_2z$ are real. Hence ${}^*zH_2z = 0$ for all z and $H_2 = 0$. Thus, if ${}^*zAz$ is real for all z, then A is hermitian. A fortiori, if A is positive definite over the complex field, it is hermitian. In particular, if a real matrix is positive definite over the <u>complex</u> <u>numbers</u>, then the matrix is symmetric.

There exist, however, non-symmetric real matrices positive definite over the real numbers. For example, $\begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix} + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \begin{pmatrix} 2 & 2 \\ 0 & 1 \end{pmatrix}$ is positive definite over the real numbers since $\begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}$ is positive definite and for all skew-symmetric matrices Q, ${}^txQx = 0$ for all x.

If a real non-symmetric matrix is positive definite over the real numbers, it is <u>not</u> positive definite over the complex numbers.

11. If U is a unitary matrix, i.e., ${}^*U \cdot U = I$, then f(U) is orthogonal since $f({}^*U \cdot U) = {}^tf(U) \cdot f(U) = I$.

12. It is well known that[10] if H is a hermitian matrix, then there exists a unitary matrix U such that ${}^*U \cdot H \cdot U$ is diagonal. Application of f yields that ${}^tf(U) \cdot f(H) \cdot f(U)$ is diagonal with f(U) orthogonal. Thus the eigenvalues of f(H) are precisely the eigenvalues of H with doubled multiplicity. In particular, it follows that $|f(H)| = |H|^2$.

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[10] Cf. Halmos, Finite Dimensional Vector Spaces, p. 129.

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